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13. ABSTRACT

The output of an industrial plant (such as a chemical plant) will in general depend on "plant conditions" i.e., factors characterizing the process such as the temperatures at which stages of the process are run, the concentrations at which chemicals are applied, the concentrations at which catalysts are used, etc. In order to "improve" such a process, it is desirable to estimate the functional dependence of the target output y on the plant conditions denoted by $x_1, x_2, \ldots, x_n$. For this purpose is it customary to use data from a planned experiment usually using a "pilot plant" in which the plant conditions x_i are deliberately determined by the experimentor in accordance with an experimental design. In such situations the plant conditions at which the pilot plant is run are often "optimized". The criterion of optimization here used is the "generalized variance" of the estimated coefficients occuring in the mathematical law representing the dependence of the output on the inputs. The particular type of experimental design considered in this technical report are, however, restricted to satisfy a well established pattern known under the name of a "Composite Design" and the parameters describing such a composite design are optimized in the sense of minimizing the generalized variance.

The composite designs considered are both of a symmetrical and asmetrical type and may or may not involve the use of fractional factorials.

ATTACHMENT 1?

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COMPOSITE DESIGNS AND THEIR OPTIMIZATION

by

James M. Lucas and H. O. Hartley

Texas A&M Research Foundation
Office of Naval Research
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ATTACHMENT I

COMPOSITE DESIGNS AND THEIR OPTIMIZATION

by

James M. Lucas and H.O. Hartley

THEMIS OPTIMIZATION RESEARCH PROGRAM
Technical Report No. 38
July 1972

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COMPOSITE DESIGNS AND THEIR OPTIMIZATION

1.1 Introduction

An important problem in industry is the improvement (which will hopefully lead to the optimization) of a process. This report attacks a problem in this area.

To improve an "ongoing process" often it is desired to examine the relationship between variables in a process, say between a y variable when y represents a "response" variable and $x_1, x_2, \ldots, x_n$, where the x's represent "input" or "control" variables. In this report we develop optimum composite designs for fitting a quadratic response surface under the standard regression assumptions, and solve some related design of experiments problems. The optimization criterion we use is the minimization of the generalized variance (the $|X'X|$ criterion).

To clarify the concept of an ongoing process we may appropriately think of a production process in a chemical plant producing a target output y of a chemical. It is commonplace that this output will depend on "plant conditions", i.e., factors characterizing the process such as the temperatures at which stages of the process are run, the concentrations at which chemicals are input, the concentrations at which catalysts are used, etc. In order to "improve" such a process, it is desirable to estimate the functional dependence of the target output y on the plant conditions denoted by $x_1, x_2, \ldots, x_n$. The data available for such an improvement may be of essentially two kinds:

(a) We may have "plant data" in which the target output y is observed along with measured records of the plant conditions $x_1, x_2, \ldots, x_n$, or

(b) We may have data from planned experiments usually us using a "pilot plant" in which the plant conditions

x_i are deliberately determined by the experimenter in accordance with an experimental plan, after which the associated target output y of the pilot plant is measured.

The concept of using an experimental design to estimate the mathematical relationship between the target output and plant conditions is normally restricted to case (b) above.
This report will be exclusively concerned with case (b). More specifically, this report is concerned with choosing the set of plant conditions, x_i, at which the pilot plant is to be run, called the experimental design, in such a manner that certain features of the mathematical relationship can be estimated with "optimum" precision. We shall confine our study to a situation in which the mathematical relationship is postulated to be of "second order", i.e., what is known as a "quadratic response surface".
It will be assumed that the expected yield of the pilot plant will be given by such a response surface and that the observed target outputs will differ from their expectations by independent equal variance residuals. These assumptions are the standard ones in "regression analysis". Using the estimation procedures appropriate to such assumptions will result in estimates of the so-called regression coefficients, i.e., effect coefficients of the x_i, their products, and squares. An estimate of the individual variances of such estimates as well as of the so-called generalized

variance of the coefficients can also be obtained. The magnitude of this generalized variance will depend on the experimental design chosen. The objective of the optimization of the design will be the minimization of this generalized variance.

The problem of the optimization of experimental designs by the minimization of the generalized variance can be reduced to a mathematical programming problem which is solved on a high speed computer. This approach was taken by Hartley and Ruud [1969] and by Crowell [1971]. The disadvantage of this attack is the complexity of the programming problem; it is generally a non-linear non-convex programming problem. Thus a global optimum cannot be guaranteed.

By restricting our attention to composite designs we will be able to avoid formulating a programming problem. We will attack the problem directly and will minimize the generalized variance for composite designs restricted to an n dimensional hypercube where n is the number of variables under study. The minimization of the generalized variance is equivalent to the maximization of $|X'X|$ where X is a $N \times p$ "expanded" design matrix having N rows and p columns, one column for each coefficient to be estimated. The $X_{N\times p}$ matrix is expanded from the design matrix X_D, a $N \times n$ matrix, which has one column for each variable under study. For a full quadratic model $p = (n+1)(n+2)/2 = 1 + n + n + \binom{n}{2}$. In the X matrix there is one column for the constant term, n for

the linear terms, n for the quadratic terms, and $\binom{n}{2}$ columns for the interaction terms.

Four types of composite designs will be examined:

(1) A "symmetric" composite design (a "symmetric" composite design has "star" point distance equal to $\pm\alpha$).

(2) A "symmetric" smallest composite design (a saturated design for which $N = p = (n+1)(n+2)/2$).

(3) An unsymmetric composite design (an unsymmetric composite design has "star" point distance equal to $(+1, -\alpha)$).

(4) An unsymmetric smallest composite design.

Composite designs are used primarily in "response surface analysis". Box and Wilson's [1951] paper opened this important and practical field, and Box and Draper's [1959] paper discussed some optimization problems in this area. Hartley and Ruud [1969] and Crowell [1971] give a good introduction to the field of optimal experimental designs and contain additional references.

1.2 Optimization of Symmetric Composite Designs

1.2.1 Alias structure I = ABCDE

A symmetric composite in n variables which is used to estimate all terms in a quadratic response surface consists of:

(1) A proper fraction (say a $1/2^k$ fraction) of a 2^n factorial array. This array of 2^{n-k} points will be placed on a hypercube having sides of length two centered at $(0, 0, \ldots, 0)_{1\times n}$.

(2) r center points.

(3) Two "star" points, one at $+\alpha$ and one at $-\alpha$, for each variable; 2n points in all.

Thus, the design consists of $N = 2^{n-k} + 2n + r$ points to estimate $p = (n+1)(n+2)/2$ terms. Table 1.1 lists the composite designs for $n \leq 11$.

We are now ready to state and prove Theorem 1.2.

Theorem 1.2: For a "symmetric" composite design the generalized variance decreases with increasing α where α is the star point distance. In this section we prove the result for alias structure such that two factor interactions are aliased with three or higher order interactions (I = ABCDE), and in the next section we indicate the changes necessitated by other alias structures.

Method of Proof:

Step 1. Indicate the structure of the $X_{N\times p}$ matrix.

Step 2. Write out the $X'X_{p\times p}$ matrix.

Step 3. Solve for $|X'X|$ and show $|X'X|$ is an increasing function of α.

Table 1.1

Common Symmetric Composite Designs

Variables	Terms in Quadratic Model	Points in Design (With one center point)	Star and Center Point	Fractional Factorial
2	6	9	5	$2^2 = 4$
3	10	15	7	$2^3 = 8$
* 3	10	11	7	$2^{3-1} = 4$
4	15	25	9	$2^4 = 16$
* 4	15	17	9	$2^{4-1} = 8$
5	21	43	11	$2^5 = 32$
5	21	27	11	$2^{5-1} = 16$
6	28	77	13	$2^6 = 64$
6	28	45	13	$2^{6-1} = 32$
* 6	28	29	13	$2^{6-2} = 16$
7	36	143	15	$2^7 = 128$
7	36	79	15	$2^{7-1} = 64$
* 7	36	47	15	$2^{7-2} = 32$
8	45	273	17	$2^8 = 256$
8	45	145	17	$2^{8-1} = 128$
8	45	81	17	$2^{8-2} = 64$
9	55	531	19	$2^9 = 512$
9	55	275	19	$2^{9-1} = 256$

Table 1.1 (Continued)

Common Symmetric Composite Designs

Variables	Terms in Quadratic Model	Points in Design (With one center point)	Star and Center Point	Fractional Factorial
9	55	147	19	$2^{9-2} = 128$
* 9	55	83	19	$2^{9-3} = 64$
10	66	1045	21	$2^{10} = 1024$
10	66	533	21	$2^{10-1} = 512$
10	66	277	21	$2^{10-2} = 256$
10	66	149	21	$2^{10-3} = 128$
11	78	2071	23	$2^{11} = 2048$
11	78	1047	23	$2^{11-1} = 1024$
11	78	535	23	$2^{11-2} = 512$
11	78	279	23	$2^{11-3} = 256$
11	78	151	23	$2^{11-4} = 128$

*The starred designs will have some three character words in an alias set (I = ABC). For all other designs it is possible to pick the alias structure so that all words in an alias set have at least five characters (I = ABCDE).

Step 1. By showing the structure of the X matrix for the i^{th} and j^{th} variables we indicate its general structure.

$$
\begin{array}{l|cccccc|}
\text{Number of Points} & u & x_i & x_i^2 & x_j & x_j^2 & x_ix_j \\
\hline
 & 1 & 1 & 1-c & 1 & 1-c & 1 \\
2^{n-k} & 1 & 1 & 1-c & -1 & 1-c & -1 \\
 & 1 & -1 & 1-c & 1 & 1-c & -1 \\
 & 1 & -1 & 1-c & -1 & 1-c & 1 \\
 & 1 & \alpha & \alpha^2-c & 0 & -c & 0 \\
4 & 1 & -\alpha & \alpha^2-c & 0 & -c & 0 \\
 & 1 & 0 & -c & \alpha & \alpha^2-c & 0 \\
 & 1 & 0 & -c & -\alpha & \alpha^2-c & 0 \\
r + 2n - 4 & 1 & 0 & -c & 0 & -c & 0 \\
\hline
\end{array}
$$

$$c = \frac{2^{n-k} + 2\alpha^2}{2^{n-k} + 2n + r}$$

c is chosen to simplify the X'X matrix. Substracting a constant from a variable does not change the value of the generalized variance as we show in Section 1.6.1 when we extend a result due to Hartley and Ruud [1969].

Step 2. By showing the structure of the $X'X_{p\times p}$ matrix for the same variables that we used in showing the structure of the $X_{N\times p}$ matrix we indicate its general structure.

Structure of $X'X_{p\times p}$ Matrix

$$
\begin{array}{c}
 \\ u \\ x_i \\ x_j \\ x_i x_j \\ x_i^2 \\ x_j^2
\end{array}
\begin{array}{c}
\begin{array}{cccccc} u & x_i & x_j & x_i x_j & x_i^2 & x_j^2 \end{array} \\
\begin{bmatrix}
2^{n-k}+2n+r & 0 & 0 & 0 & 0 & 0 \\
0 & 2^{n-k}+2\alpha^2 & 0 & 0 & 0 & 0 \\
0 & 0 & 2^{n-k}+2\alpha^2 & 0 & 0 & 0 \\
0 & 0 & 0 & 2^{n-k} & 0 & 0 \\
0 & 0 & 0 & 0 & ** & * \\
0 & 0 & 0 & 0 & * & **
\end{bmatrix}
\end{array}
$$

where

$$** = 2^{n-k}(1-c)^2 + 2(\alpha^2-c)^2 + (r+2n-2)\ c^2$$

$$* = 2^{n-k}(1-c)^2 - 4c(\alpha^2-c) + (r+2n-4)\ c^2$$

Step 3. The $X'X_{p\times p}$ matrix is a diagonal matrix except for an $n\times n$ matrix which has the structure

$$[aI + bJJ']_{n\times n} = [M]$$

where

$$a = 2(\alpha^2-c)^2 + 2c^2 + 4c(\alpha^2-c) = 2\alpha^4$$

$$b = 2^{n-k}(1-c)^2 + (r+2n-4)\ c^2 - 4c(\alpha^2-c)$$

I is an $n\times n$ identity matrix, and

J is a n vector of ones .

Thus

$$|X'X| = (2^{n-k}+2n+r)(2^{n-k}+2\alpha^2)^n(2^{n-k})^{\binom{n}{2}}|M| \quad .$$

We show in the Appendix, Theorem [4], that

$$|M| = a^n + na^{n-1}b = a^{n-1}(a+nb) \quad .$$

Substituting a, b, and c in $|M|$ we find

$$|M| = (2\alpha^4)^{n-1}\frac{1}{(2^{n-k}+2n+r)}\left\{(2^{n-k+1}+2r)\alpha^4 - n2^{n-k+2}\ \alpha^2 + n2^{n-k}(2n+r)\right\}.$$

Thus

$$|X'X| = 2^{2n-1}(2^{n-k})^{\binom{n}{2}}(2^{n-k-1}+\alpha^2)^n(\alpha^{4(n-1)})$$

$$\{2^{n-k+1}(\alpha^2-n)^2 + 2r\alpha^4 + nr2^{n-k}\} \quad .$$

To show that this is an increasing function we take the logarithm, differentiate it, and show that the derivative has no positive zeros. This will show that $|X'X|$ is a product of increasing functions, and so is an increasing function of α.

$$\log\ |X'X| = K + n\ \log(2^{n-k-1}+\alpha^2) + 4(n-1)\ \log\ \alpha$$

$$+ \log\ \{(\alpha^2-n)^2 + \frac{r\alpha^4}{2^{n-k}} + \frac{nr}{2}\}$$

$$\frac{d\ \log\ |X'X|}{d\alpha} = \frac{2n\alpha}{2^{n-k-1}+\alpha^2} + \frac{4(n-1)}{\alpha}$$

$$+ \left\{\frac{4\ (\alpha^2-n) + r\alpha^3/2^{n-k-2}}{(\alpha^2-n)^2 + r\alpha^4/2^{n-k} + nr/2}\right\} \quad .$$

Combining fractions using the last two terms only, we obtain a numerator greater than:

$$2n\,[2\alpha^4 - (4n-2)\,\alpha^2 + 2n^2 - n - 1] \quad .$$

The discriminant of the term in brackets is $4(-2n+3)$. Thus for $n > 1$, $d \log |X'X|/d\alpha$ is nowhere negative, and $|X'X|$ is increasing with α. $n=1$ is an easy special case for which it is trivial to show that $|X'X|$ is increasing with α so the result holds for all n.

The preceding shows that the optimal symmetric composite design on a hypercube with sides of length two centered at the origin has $\alpha = 1.0$.

In Section 1.6.1 we show that expanding the hypercube by a factor k introduces a multiplying factor $k^{2n(n+2)}$ to the determinant. A ξ increase in the size of the hypercube gives a multiplying factor of $(1 + 2n(n+2)\,\xi)$ to the determinant when we consider only first order terms. For an ξ increase in α from 1 to $1+\xi$ a multiplying factor for the determinant of $(1 + 6n\xi)$ is obtained. Thus, for optimal composite designs on a hypercube we need only consider fractional factorials with points at the extremes of the hypercube. Similar considerations hold for the fractional factorial portion of all designs considered in this chapter. The above result can be found in Box and

Draper [1971]. This publication came out after we had independently obtained the same result. They do not note that this form of $|X'X|$ does not hold for all alias structures. We discuss this in the next section of our paper.

1.2.2 Other alias structures

With other alias structures it may not be possible to estimate all terms in a quadratic model. The estimable terms can be found using Theorem 1 of Hartley [1959] which we discuss and extend in Section 1.6. For alias structure I = ABCD the proof goes through exactly as given except that three of the product terms cannot be estimated.

The I = ABC alias structure is a good one in that it allows the estimation of all coefficients of a quadratic response surface. For a six row, six column minor of the determinant with alias structure I = ABC we obtain:

$$\begin{array}{c c}
 & \begin{array}{cccccc} a & b & c & bc & ac & ab \end{array} \\
\begin{array}{c} a \\ b \\ c \\ bc \\ ac \\ ab \end{array} &
\begin{bmatrix}
2^{n-k}+2\alpha^2 & 0 & 0 & 2^{n-k} & 0 & 0 \\
0 & 2^{n-k}+2\alpha^2 & 0 & 0 & 2^{n-k} & 0 \\
0 & 0 & 2^{n-k}+2\alpha^2 & 0 & 0 & 2^{n-k} \\
2^{n-k} & 0 & 0 & 2^{n-k} & 0 & 0 \\
0 & 2^{n-k} & 0 & 0 & 2^{n-k} & 0 \\
0 & 0 & 2^{n-k} & 0 & 0 & 2^{n-k}
\end{bmatrix}
\end{array}$$

With alias structure I = ABCDE the off-diagonal elements would not be obtained. For this minor the determinant is $(2^{n-k+1}\,\alpha^2)^3$. This increasing function of α substitutes for $(2^{n-k}+2\alpha^2)^3\,2^{3(n-k)}$ obtained with alias structure I = ABCDE. Otherwise, the argument is unchanged.

For the I = A alias structure we choose a subtraction constant b to make the X_a column orthogonal to the X_a^2 column and note that this choice of b makes the X_a column orthogonal to every column except the column for the constant terms.

$$b = \frac{2^{n-k}(1-c)}{2^{n-k}(1-c) + 2\alpha^2 - (2n+r)\,c}$$

and the changed minor in the X'X matrix is

$$\begin{array}{cc} & \begin{array}{cc} u & X_a \end{array} \\ \begin{array}{c} u \\ X_a \end{array} & \begin{bmatrix} 2^{n-k} + 2n + r & 2^{n-k} - (2^{n-k}+2n+r)b \\ 2^{n-k} - (2^{n-k}+2n+r)b & (2^{n-k}+2n+r)b^2 + 2^{n-k+1}b + 2^{n-k} + 2\alpha^2 \end{bmatrix} \end{array}$$

This minor has determinant

$$2^{n-k}(2n+r) + (2^{n-k}+2n+r)\,2\alpha^2$$

an increasing function of α.

The $I = AB$ alias structure is not recommended for $n > 2$ since all terms in a quadratic model cannot be estimated. $I = AB$ implies $AC = BC$ and only one of the pair of interactions can be included in the model. Two minors are changed by this alias structure. They are:

$$\begin{array}{c} \\ 1 \\ X_aX_b \end{array} \begin{array}{c} \begin{array}{cc} u & X_aX_b \end{array} \\ \begin{bmatrix} 2^{n-k}+2n+r & 2^{n-k} \\ 2^{n-k} & 2^{n-k} \end{bmatrix} \end{array} \qquad \begin{array}{c} \\ X_a \\ X_b \end{array} \begin{array}{c} \begin{array}{cc} X_a & X_b \end{array} \\ \begin{bmatrix} 2^{n-k}+2\alpha^2 & 2^{n-k} \\ 2^{n-k} & 2^{n-k}+2\alpha^2 \end{bmatrix} \end{array}$$

with determinants

$$2^{n-k}(2n+r) \quad \text{and} \quad 2^{n+k+2}\,\alpha^2 + 4\alpha^4 \quad .$$

So an increasing function of α is obtained.

1.3 Optimization of Smallest Composite Designs Symmetric in the Star Points

By using an improper fraction of a 2^n factorial array we can estimate all terms in a quadratic model using fewer experimental points than we need if we use a proper fraction of a 2^n factorial array. A smallest composite design is obtained when we have a saturated design, i.e., when we have exactly as many points in

the design as we have regression coefficients to be estimated. To estimate all terms in a quadratic response surface in n variables we need $p = (n+1)(n+2)/2$ points to estimate the p terms in the model. Small designs like this are used when experimentation is expensive, experimental error is small, an independent estimate of experimental error is available, and a quadratic model is adequate to explain the phenomena under study. These designs have a variance structure for the regression coefficients that is worse than the variance structure for balanced designs; they give no estimate of the experimental error; and they can give no test of the adequacy of the model. For smallest composite designs symmetric in the star points, we now follow exactly the same procedure used in Section 1.2.

A smallest composite design symmetric in the star points consists of:

1. An edge point having the structure

$$\begin{array}{c} (0 \;\ldots\; 010 \;\ldots\; 010 \;\ldots\; 0)_{1\times n} \\ 1 \;\ldots\; i \;\ldots\; j \;\ldots\; n \end{array} \quad .$$

   It is a vector having 1's in the i^{th} and j^{th} location and zeros elsewhere. This point enables the estimation of the $x_i x_j$ (two factor interactions) term in the quadratic model. We need one edge point for each interaction term desired in the model. If all interaction

terms are to be estimated there will be $\binom{n}{2} = n(n-1)/2$ points of this type.

2. One center point.

3. Two star points, one at $+\alpha$ and one at $-\alpha$, for each variable.

<u>Theorem 1.3</u>: For a smallest composite design symmetric in the star points that is used to estimate a quadratic response surface, the generalized variance decreases with increasing α. The method of proof follows the same three steps used in Theorem 1.2.

Step 1. We write down the $N \times n$ design matrix X_D which is "expanded" to give the X matrix.

$$
\begin{array}{cc}
 & \begin{array}{ccccc} x_1 & x_2 & x_3 & \cdots & x_n \end{array} \qquad \text{Number of Points} \\
X_D = &
\left[\begin{array}{ccccc}
1 & 1 & 0 & \cdots & 0 \\
1 & 0 & 1 & \cdots & 0 \\
0 & 1 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & 1 \\
\alpha & 0 & 0 & \cdots & 0 \\
-\alpha & 0 & 0 & \cdots & 0 \\
0 & \alpha & 0 & \cdots & 0 \\
0 & -\alpha & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & \alpha \\
0 & 0 & 0 & \cdots & -\alpha \\
0 & 0 & 0 & \cdots & 0
\end{array}\right]
\begin{array}{l}
\left.\begin{array}{l} \\ \\ \\ \\ \\ \end{array}\right\} S \le \binom{n}{2} \\
\left.\begin{array}{l} \\ \\ \\ \\ \\ \\ \\ \end{array}\right\} 2n \\
\quad 1
\end{array}
\end{array}
$$

We first prove the result for the case $S = \binom{n}{2}$, when all interactions are to be estimated.

Step 2. The [X'X] matrix is:

$$
\begin{array}{c}
\\
u \\ x_1 \\ x_2 \\ \vdots \\ x_n \\ x_1^2 \\ x_2^2 \\ \vdots \\ x_n^2 \\ x_1x_2 \\ x_1x_3 \\ \vdots \\ x_{n-1}x_n
\end{array}
\begin{array}{c}
\begin{array}{cccccccccc}
u & x_1 & x_2 & \cdots & x_n & x_1^2 & x_2^2 & \cdots & x_n^2 & x_1x_2\ x_1x_3 \cdots x_{n-1}x_n
\end{array}
\\
\left[\begin{array}{c|cccc|cccc|c}
1+2n+\binom{n}{2} & n-1 & n-1 & \cdots & n-1 & n-1+2\alpha^2 & n-1+2\alpha^2 & \cdots & n-1+2\alpha^2 & J_{\binom{n}{2}\times 1}' \\
\hline
n-1 & n-1+2\alpha^2 & 1 & \cdots & 1 & n-1 & 1 & \cdots & 1 & \\
n-1 & 1 & n-1+2\alpha^2 & \cdots & 1 & 1 & n-1 & \cdots & 1 & A' \\
\vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \\
n-1 & 1 & 1 & \cdots & n-1+2\alpha^2 & 1 & 1 & \cdots & n-1 & \\
\hline
n-1+2\alpha^2 & n-1 & 1 & \cdots & 1 & n-1+2\alpha^4 & 1 & \cdots & 1 & \\
n-1+2\alpha^2 & 1 & n-1 & \cdots & 1 & 1 & n-1+2\alpha^4 & \cdots & 1 & A' \\
\vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \\
n-1+2\alpha^2 & 1 & 1 & \cdots & n-1 & 1 & 1 & \cdots & n-1+2\alpha^4 & \\
\hline
 & & & & & & & & & \\
 & & & & & & & & & \\
J_{\binom{n}{2}\times 1} & \multicolumn{4}{c|}{A} & \multicolumn{4}{c|}{A} & I_{\binom{n}{2}\times\binom{n}{2}} \\
 & & & & & & & & &
\end{array}\right]
\end{array}
$$

where

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 1 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}_{\binom{n}{2}\times n}$$

Step 3. Solve for the determinant of the X'X matrix. We know that

$$|X'X| = \begin{vmatrix} D & B' \\ B & C \end{vmatrix} = |C|\,|D - B'C^{-1}B| \quad .$$

Using the above with $C = I_{\binom{n}{2}\times\binom{n}{2}}$ so $|C| = 1$, we obtain

$$B'C^{-1}B = \begin{bmatrix} J' \\ A' \\ A' \end{bmatrix} [I] \quad [J \mid A \mid A]$$

$$= \begin{bmatrix}
\binom{n}{2} & n-1 & n-1 & \cdots & n-1 & n-1 & n-1 & \cdots & n-1 \\
n-1 & n-1 & 1 & \cdots & 1 & n-1 & 1 & \cdots & 1 \\
n-1 & 1 & n-1 & \cdots & 1 & 1 & n-1 & \cdots & 1 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
n-1 & 1 & 1 & \cdots & n-1 & 1 & 1 & \cdots & n-1 \\
n-1 & n-1 & 1 & \cdots & 1 & n-1 & 1 & \cdots & 1 \\
n-1 & 1 & n-1 & \cdots & 1 & 1 & n-1 & \cdots & 1 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
n-1 & 1 & 1 & \cdots & n-1 & 1 & 1 & \cdots & n-1
\end{bmatrix}_{(2n+1)\times(2n+1)}$$

Thus

$$|X'X| = |D - B' C^{-1} B| =$$

$$\begin{bmatrix}
1+2n & 0 & 0 & \cdots & 0 & 2\alpha^2 & 2\alpha^2 & \cdots & 2\alpha^2 \\
0 & 2\alpha^2 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 2\alpha^2 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\
2\alpha^2 & 0 & 0 & \cdots & 2\alpha^2 & 0 & 0 & \cdots & 0 \\
2\alpha^2 & 0 & 0 & \cdots & 0 & 2\alpha^4 & 0 & & 0 \\
\vdots & \vdots & \vdots & & \vdots & 0 & 2\alpha^4 & & 0 \\
 & & & & & & & \ddots & \\
2\alpha^2 & 0 & 0 & \cdots & 0 & 0 & 0 & & 2\alpha^4
\end{bmatrix}$$

which upon using Theorem [1] again is

$$(2\alpha^2)^n(2\alpha^4)^n[1 + 2n - \frac{1}{2\alpha^4} n4\alpha^4] = 2^{2n} \alpha^{6n}$$

which is an increasing function of α.

If $S < \binom{n}{2}$ interactions are to be estimated, exactly the same determinant is obtained. This can be seen by induction. If one interaction vector is removed from the X matrix, we can use exactly the same proof and note that the determinant does

not change. Similarly, we can note that if (k-1) interaction vectors are removed, the value of the determinant will not be changed by the removal of the k^{th} vector. This procedure enables us to remove all undesirable interactions terms until we have left only the S interaction terms which we wish to estimate.

If the design is restricted to a hypercube having sides of length two centered at the origin, the above immediately gives the optimum value of α as $\alpha = 1$.

1.4 Optimization of Smallest Composite Designs Unsymmetric in the Star Points

A smallest composite design unsymmetric in the star points differs from a smallest composite design symmetric in the star points in that the star points are placed at +1 and $-\alpha$ in the unsymmetric design rather than at $\pm\alpha$ as is the case for the design symmetric in the star points.

Theorem 1.4: For a smallest composite design unsymmetric in the star points, the generalized variance decreases with increasing α. When the design is restricted to a hypercube having sides of length one (which makes the star point distance $\alpha/(1+\alpha)$), the optimum star point distance is $1/(n+1)$.

The first part of the theorem is proved following the same steps used previously.

Step 1.

$$
\begin{array}{ccc}
 & \begin{array}{ccccc} x_1 & x_2 & x_3 & \cdots & x_n \end{array} & \text{Number of Points} \\
X_D = & \left[\begin{array}{ccccc}
1 & 1 & 0 & \cdots & 0 \\
1 & 0 & 1 & \cdots & 0 \\
0 & 1 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & 1 \\
1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 1 & \cdots & 0 \\
 & & & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 1 \\
-\alpha & 0 & 0 & \cdots & 0 \\
0 & -\alpha & 0 & \cdots & 0 \\
0 & 0 & -\alpha & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & -\alpha \\
0 & 0 & 0 & \cdots & 0
\end{array}\right] &
\begin{array}{l}
\left.\vphantom{\begin{array}{c}1\\1\\0\\\vdots\\0\end{array}}\right\} S \le \binom{n}{2} \\
\left.\vphantom{\begin{array}{c}1\\0\\0\\\ddots\\0\end{array}}\right\} n \\
\left.\vphantom{\begin{array}{c}1\\0\\0\\\vdots\\0\end{array}}\right\} n \\
\quad 1
\end{array}
\end{array}
$$

Step 2. $[X'X] =$

$$
\begin{array}{cc}
 & \begin{array}{ccccccccccccc} u & x_1 & x_2 & \cdots & x_n & x_1^2 & x_2^2 & \cdots & x_n^2 & x_1x_2 & x_1x_3 & \cdots & x_{n-1}x_n \end{array} \\
\begin{array}{c} u \\ x_1 \\ x_2 \\ \vdots \\ x_n \\ x_1^2 \\ x_2^2 \\ \vdots \\ x_n^2 \\ x_1x_2 \\ x_1x_3 \\ \vdots \\ x_{n-1}x_n \end{array} &
\left[\begin{array}{ccccccccccccc}
1+2n+\binom{n}{2} & n-\alpha & n-\alpha & \cdots & n-\alpha & n+\alpha^2 & n+\alpha^2 & \cdots & n+\alpha^2 & & J' & & \\
n-\alpha & n+\alpha^2 & 1 & \cdots & 1 & n-\alpha^3 & 1 & \cdots & 1 & & & & \\
n-\alpha & 1 & n+\alpha^2 & \cdots & 1 & 1 & n-\alpha^3 & \cdots & 1 & & A' & & \\
 & \vdots & \vdots & \ddots & & \vdots & \vdots & \ddots & & & & & \\
n-\alpha & 1 & 1 & & n+\alpha^2 & 1 & 1 & & n-\alpha^3 & & & & \\
n+\alpha^2 & n-\alpha^3 & 1 & \cdots & 1 & n+\alpha^4 & 1 & \cdots & 1 & & & & \\
n+\alpha^2 & 1 & n-\alpha^3 & \cdots & 1 & 1 & n+\alpha^4 & \cdots & 1 & & A' & & \\
\vdots & \vdots & \vdots & \ddots & & \vdots & \vdots & \ddots & \vdots & & & & \\
n+\alpha^2 & 1 & 1 & & n-\alpha^3 & 1 & 1 & \cdots & n+\alpha^4 & & & & \\
 & & & & & & & & & & & & \\
J & & A & & & & A & & & & I_{\binom{n}{2}\times\binom{n}{2}} & & \\
 & & & & & & & & & & & & \\
 & & & & & & & & & & & &
\end{array}\right]
\end{array}
$$

where J, A, and I are the same as they were in Section 1.3.

Using

$$\begin{vmatrix} D & B' \\ B & C \end{vmatrix} = |C| \quad |D - B\ C^{-1}\ B|$$

we obtain

$[D - B'\ C^{-1}\ B]$

$$\begin{bmatrix}
1+2n & 1-\alpha & 1-\alpha & \cdots & 1-\alpha & 1+\alpha^2 & 1+\alpha^2 & \cdots & 1+\alpha^2 \\
1-\alpha & 1+\alpha^2 & 0 & \cdots & 0 & 1-\alpha^3 & 0 & \cdots & 0 \\
1-\alpha & 0 & 1+\alpha^2 & \cdots & 0 & 0 & 1-\alpha^3 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
1-\alpha & 0 & 0 & \cdots & 1+\alpha^2 & 0 & 0 & \cdots & 1-\alpha^3 \\
1+\alpha^2 & 1-\alpha^3 & 0 & \cdots & 0 & 1+\alpha^4 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
1+\alpha^2 & 0 & 0 & \cdots & 1-\alpha^3 & 0 & 0 & \cdots & 1+\alpha^4
\end{bmatrix}$$

We use the same breakdown we used before letting $D_{1\times 1} = 1+2n$ so C is a $2n\times 2n$ matrix. Using Theorem [6] with $b = d = f = 0$ we obtain

$$|C| = [(1+\alpha^2)(1+\alpha^4) - (1-\alpha^3)^2]^n$$

$$= \alpha^{2n}(1+\alpha)^{2n}$$

$$[C]^{-1} = \frac{1}{(1+\alpha^2)(1+\alpha^4)-(1-\alpha^3)^2} \begin{bmatrix} (1+\alpha^4)\ I_{n\times n} & -(1-\alpha^3)\ I_{n\times n} \\ -(1-\alpha_3)\ I_{n\times n} & (1+\alpha^2)\ I_{n\times n} \end{bmatrix}$$

then

$$|D - B'\ C^{-1}\ B| = 1 + 2n - \frac{1}{\alpha^2(1+\alpha^2)} \begin{bmatrix} (1-\alpha)\ J'_{n\times 1} & (1+\alpha^2)\ J'_{n\times 1} \end{bmatrix}$$

$$\begin{bmatrix} (1+\alpha^4)\ I_{n\times n} & -(1-\alpha^3)\ I_{n\times n} \\ -(1-\alpha^3)\ I_{n\times n} & (1+\alpha^4)\ I_{n\times n} \end{bmatrix} \begin{bmatrix} (1-\alpha)\ J_{n\times 1} \\ (1+\alpha^2)\ J_{n\times 1} \end{bmatrix}$$

$$= 1 \quad .$$

So $|X'X| = \alpha^{2n}(1+\alpha)^{2n}$. By the same type of argument used in Section 1.3, the determinant has the same value for all $S \leq \binom{n}{2}$. Thus, the determinant is an increasing function of α.

To complete this proof we show that if this design is

restricted to a hypercube having sides of length one, the optimum star point distance is $1/(n+1)$. For this proof we need an extension of a result due to Hartley and Ruud [1969], which we discuss in Section 1.6. Restricting the design to a hypercube having sides of lengths one introduces a multiplier for the determinant of $k^{2n(n+2)}$ where $k = 1/(1+\alpha)$. Thus the determinant of the restricted X'X matrix is

$$|X'X|_{\text{restricted}} = \frac{1}{(1+\alpha)^{2n(n+2)}} \alpha^{2n}(1+\alpha)^{2n} = \frac{\alpha^{2n}}{(1+\alpha)^{2n(n+1)}}$$

thus

$$\frac{d|X'X|}{d\alpha} = \frac{2n\alpha^{2n-1}(1+\alpha)^{2n(n-1)} - 2n(n+1)(1+\alpha)^{2n(n+1)-1}\alpha^{2n}}{(1+\alpha)^{4n(n+1)}} = 0$$

$$\Rightarrow \qquad (1+\alpha) - (n+1)\alpha = 0$$

$$\Rightarrow \qquad \alpha = 1/n$$

where $0 < \alpha < \infty$. We must transform this to the proper units. Since the length of the design $1 + \alpha$ is restricted to be one, the optimal star point distance is

$$\frac{\alpha}{1+\alpha} = \frac{1/n}{1+1/n} = \frac{1}{n+1} \quad .$$

To obtain the optimum star point distance by another method, we reprove the second part of the theorem by rescaling the determinant before we differentiate to solve for the optimum star point distance. Let β be the star point distance, then

$$\frac{\alpha}{1} = \frac{\beta}{1-\beta}$$

so

$$1+\alpha = 1/(1-\beta)$$

$$k = (1-\beta)$$

and

$$|X'X|_{\text{restricted}} = \left(\frac{\beta}{1-\beta}\right)^{2n}\left(\frac{1}{1-\beta}\right)^{2n}(1-\beta)^{2n(n+2)} = \beta^{2n}(1-\beta)^{2n^2}$$

$$\frac{d|X'X|_{\text{restricted}}}{d\beta} = 2n\beta^{2n-1}(1-\beta)^{2n^2} - 2n^2\,\beta^{2n}(1-\beta)^{2n^2-1} = 0$$

$$\Rightarrow \qquad (1-\beta) - n\beta = 0$$

$$\Rightarrow \qquad \beta = 1/(n+1) \quad .$$

A third method of finding the optimum star point distance is to rescale the design matrix, then optimize it following the three steps indicated previously.

Step 1. We show the structure of the design matrix X_D:

$$
\begin{array}{ccl}
 & \begin{array}{ccccc} x_1 & x_2 & x_3 & \cdots & x_n \end{array} & \text{Number of Points} \\
X_D = & \left[\begin{array}{ccccc}
1-\beta & 1-\beta & 0 & \cdots & 0 \\
1-\beta & 0 & 1-\beta & \cdots & 0 \\
0 & 1-\beta & 1-\beta & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & 1-\beta \\
1-\beta & 0 & 0 & \cdots & 0 \\
0 & 1-\beta & 0 & \cdots & 0 \\
0 & 0 & 1-\beta & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & 1-\beta \\
-\beta & 0 & 0 & \cdots & 0 \\
0 & -\beta & 0 & \cdots & 0 \\
0 & 0 & -\beta & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots \\
0 & 0 & 0 & \cdots & -\beta \\
0 & 0 & 0 & \cdots & 0
\end{array}\right] &
\begin{array}{l}
\left.\begin{array}{c} \\ \\ \\ \\ \\ \end{array}\right\} \binom{n}{2} \\
\left.\begin{array}{c} \\ \\ \\ \\ \\ \end{array}\right\} n \\
\left.\begin{array}{c} \\ \\ \\ \\ \\ \end{array}\right\} n \\
\quad 1
\end{array}
\end{array}
$$

Step 2. We indicate the structure of the X'X matrix by showing it for selected rows and columns:

$$
\begin{array}{c}
\\
u \\ x_i \\ x_j \\ x_i^2 \\ x_j^2 \\ x_ix_j \\ x_ix_n \\ x_jx_n
\end{array}
\begin{array}{c}
\begin{array}{cccccccc}
u & x_i & x_j & x_i^2 & x_j^2 & x_ix_j & x_ix_n & x_jx_n
\end{array} \\
\begin{bmatrix}
1+2n+\binom{n}{2} & n(1-\beta)-\beta & n(1-\beta)-\beta & n(1-\beta)^2+\beta^2 & n(1-\beta)^2+\beta^2 & (1-\beta)^2 & (1-\beta)^2 & (1-\beta)^2 \\
n(1-\beta)-\beta & n(1-\beta)^2+\beta^2 & (1-\beta)^2 & n(1-\beta)^3-\beta^3 & (1-\beta)^3 & (1-\beta)^3 & (1-\beta)^3 & 0 \\
n(1-\beta)-\beta & (1-\beta)^2 & n(1-\beta)^2+\beta^2 & (1-\beta)^3 & n(1-\beta)^3-\beta^3 & (1-\beta)^3 & 0 & (1-\beta)^3 \\
n(1-\beta)^2+\beta^2 & n(1-\beta)^3-\beta^3 & (1-\beta)^3 & n(1-\beta)^4+\beta^4 & (1-\beta)^4 & (1-\beta)^4 & (1-\beta)^4 & 0 \\
n(1-\beta)^2+\beta^2 & (1-\beta)^3 & n(1-\beta)^3-\beta^3 & (1-\beta)^4 & n(1-\beta)^4+\beta^4 & (1-\beta)^4 & 0 & (1-\beta)^4 \\
(1-\beta)^2 & (1-\beta)^3 & (1-\beta)^3 & (1-\beta)^4 & (1-\beta)^4 & (1-\beta)^4 & 0 & 0 \\
(1-\beta)^2 & (1-\beta)^3 & 0 & (1-\beta)^4 & 0 & 0 & (1-\beta)^4 & 0 \\
(1-\beta)^2 & 0 & (1-\beta)^3 & 0 & (1-\beta)^4 & 0 & 0 & (1-\beta)^4
\end{bmatrix}
\end{array}
$$

using

$$\begin{vmatrix} D & B^t \\ B & C \end{vmatrix} = |C| \; |D - B^t C^{-1} B|$$

with

$$C = (1-\beta)^4 \, I_{\binom{n}{2}\times\binom{n}{2}}$$

we reduce the problem to:

$$|X'X| = (1-\beta)^{4\binom{n}{2}} \times$$

$$\begin{bmatrix}
1+2n & 1-2\beta & 1-2\beta & \cdots & 1-2\beta & (1-\beta)^2+\beta^2 & (1-\beta)^2+\beta^2 & \cdots & (1-\beta)^2+\beta^2 \\
1-2\beta & (1-\beta)^2+\beta^2 & 0 & \cdots & 0 & (1-\beta)^3-\beta^3 & 0 & \cdots & 0 \\
1-2\beta & 0 & (1-\beta)^2+\beta^2 & \cdots & 0 & 0 & (1-\beta)^3-\beta^3 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
1-2\beta & 0 & 0 & \cdots & (1-\beta)^2+\beta^2 & 0 & 0 & \cdots & (1-\beta)^3-\beta^3 \\
(1-\beta)^2+\beta^2 & (1-\beta)^3-\beta^3 & 0 & \cdots & 0 & (1-\beta)^4+\beta^4 & 0 & \cdots & 0 \\
(1-\beta)^2+\beta^2 & 0 & (1-\beta)^3-\beta^3 & \cdots & 0 & 0 & (1-\beta)^4+\beta^4 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
(1-\beta)^2+\beta^2 & 0 & 0 & \cdots & (1-\beta)^3-\beta^3 & 0 & 0 & \cdots & (1-\beta)^4+\beta^4
\end{bmatrix}$$

Reusing

$$\begin{vmatrix} D & B' \\ B & C \end{vmatrix} = |C| \; |D - B' \, C^{-1} \, B|$$

with $n = 1+2n$ obtain

$$|D - B' \, C^{-1} \, B| = 1$$

and

$$|C| = \{((1-\beta)^4+\beta^4)((1-\beta)^2+\beta^2) - ((1-\beta)^3-\beta^3)^2\}^n$$

$$= \beta^{2n}(1-\beta)^{2n}$$

so

$$|X'X| = (1-\beta)^{4\binom{n}{2}} \beta^{2n}(1-\beta)^{2n} = \beta^{2n}(1-\beta)^{2n^2}$$

which reduces the result to that of the determinant in the second alternative proof; thus $\beta = 1/(n+1)$ is optimal.

1.5 Optimization of Composite Designs Unsymmetric in the Star Points

A composite design unsymmetric in the star points consists of a proper fraction of a 2^n factorial array, and n star points.

Theorem 1.5: For a composite design unsymmetric in the star points that is used to estimate a quadratic model the generalized variance decreases with α, the star point distance. When the design is restricted to a hypercube having sides of length one, the optimal star point distance is $1/(n+1)$.

Thus even though there are many more points in the cube part of the design, the optimal star point distance is the same as that obtained for smallest composite designs unsymmetric in the star points. The proof will follow the same three steps used in the previous proofs though the algebra is more involved and more involved matrix results are used.

To prove the theorem, we reduce the determinant to a constant (independent of α) times the result for Theorem 1.4.

Possible composite designs unsymmetric in the star points for estimating a quadratic model for $n \leq 11$ are listed in Table 1.2.

Table 1.2

Common Unsymmetric Composite Designs

Variables	Terms in Quadratic Model	Points in Design	Fractional Factorial	
2	6	6	$2^2 = 4$	
3	10	11	$2^3 = 8$	
4	15	20	$2^4 = 16$	
5	21	37	$2^5 = 32$	
5	21	21	$2^{5-1} = 16$	
6	28	70	$2^6 = 64$	
6	28	38	$2^{6-1} = 32$	
7	36	135	$2^7 = 128$	
7	36	71	$2^{7-1} = 64$	
7	36	39	$2^{7-2} = 32$	*
8	45	264	$2^8 = 256$	
8	45	136	$2^{8-1} = 128$	
8	45	72	$2^{8-2} = 64$	
9	55	521	$2^9 = 512$	
9	55	265	$2^{9-1} = 256$	
9	55	137	$2^{9-2} = 128$	
9	55	73	$2^{9-3} = 64$	*
10	66	1034	$2^{10} = 1024$	
10	66	522	$2^{10-1} = 512$	

Table 1.2 (Continued)

Common Unsymmetric Composite Designs

Variables	Terms in Quadratic Model	Points in Design	Fractional Factorial
10	66	266	$2^{10-2} = 256$
10	66	138	$2^{10-3} = 128$
10	66	74	$2^{10-4} = 64$ *
11	78	2059	$2^{11} = 2048$
11	78	1035	$2^{11-1} = 1024$
11	78	523	$2^{11-2} = 512$
11	78	267	$2^{11-3} = 256$
11	78	139	$2^{11-4} = 128$

While the designs indicated with a * have more experimental points than there are parameters in a full quadratic model, the alias structure is such that all parameters in a quadratic response surface cannot be estimated. See Section 1.6.2.

Step 1. We indicate the structure of the X matrix for a number of selected variables.

u	x_i	x_j	x_k	x_e	x_i^2	x_j^2	x_k^2	x_{ij}	x_{ik}	x_{ke}	
1	1	1	1	1	1	1	1	1	1	1	
1	1	1	1	0	1	1	1	1	1	0	
1	1	1	0	1	1	1	0	1	0	0	
1	1	1	0	0	1	1	0	1	0	0	
1	1	0	1	1	1	0	1	0	1	1	
1	1	0	1	0	1	0	1	0	1	0	
1	1	0	0	1	1	0	0	0	0	0	
1	1	0	0	0	1	0	0	0	0	0	
1	0	1	1	1	0	1	1	0	0	1	2^{n-k}
1	0	1	1	0	0	1	1	0	0	0	
1	0	1	0	1	0	1	0	0	0	0	
1	0	1	0	0	0	1	0	0	0	0	
1	0	0	1	1	0	0	1	0	0	1	
1	0	0	1	0	0	0	1	0	0	0	
1	0	0	0	1	0	0	0	0	0	0	
1	0	0	0	0	0	0	0	0	0	0	
1	$-\alpha$	0	0	0	α^2	0	0	0	0	0	
1	0	$-\alpha$	0	0	0	α^2	0	0	0	0	n
1	0	0	$-\alpha$	0	0	0	α^2	0	0	0	
1	0	0	0	–	0	0	0	0	0	0	

Step 2. $[X'X] =$

$$
\begin{array}{cc}
 & \begin{array}{ccccccccccc} u & x_1 & x_2 & \cdots & x_n & x_1^2 & x_2^2 & \cdots & x_n^2 & x_1x_2 & x_1x_3 \cdots x_{n-1}x_n \end{array} \\
\begin{array}{c} u \\ x_1 \\ x_2 \\ \vdots \\ x_n \\ x_1^2 \\ x_2^2 \\ \vdots \\ x_n^2 \\ x_1x_2 \\ x_1x_3 \\ \vdots \\ x_{n-1}x_n \end{array}
&
\left[\begin{array}{cccccccccc}
2^{n-k}+n & 2^{n-k-1}-\alpha & 2^{n-k-1}-\alpha & \cdots & 2^{n-k-1}-\alpha & 2^{n-k-1}+\alpha^2 & 2^{n-k-1}+\alpha^2 & \cdots & 2^{n-k-1}+\alpha^2 & J'_{\binom{n}{2}\times 1} \\
2^{n-k-1}-\alpha & 2^{n-k-1}+\alpha^2 & 2^{n-k-2} & \cdots & 2^{n-k-2} & 2^{n-k-1}-\alpha^3 & 2^{n-k-2} & \cdots & 2^{n-k-2} & \\
2^{n-k-1}-\alpha & 2^{n-k-2} & 2^{n-k-1}+\alpha^2 & \cdots & 2^{n-k-2} & 2^{n-k-2} & 2^{n-k-1}-\alpha^3 & \cdots & 2^{n-k-2} & A'_{\binom{n}{2}\times n} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \\
2^{n-k-1}-\alpha & 2^{n-k-2} & 2^{n-k-2} & \cdots & 2^{n-k-1}+\alpha^2 & 2^{n-k-2} & 2^{n-k-2} & \cdots & 2^{n-k-1}-\alpha^3 & \\
2^{n-k-1}+\alpha^2 & 2^{n-k-1}-\alpha^3 & 2^{n-k-2} & \cdots & 2^{n-k-2} & 2^{n-k-1}+\alpha^4 & 2^{n-k-2} & \cdots & 2^{n-k-2} & \\
2^{n-k-1}+\alpha^2 & 2^{n-k-2} & 2^{n-k-1}-\alpha^3 & \cdots & 2^{n-k-2} & 2^{n-k-2} & 2^{n-k-1}+\alpha^4 & \cdots & 2^{n-k-2} & A'_{\binom{n}{2}\times n} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \\
2^{n-k-1}+\alpha^2 & 2^{n-k-2} & 2^{n-k-2} & \cdots & 2^{n-k-1}-\alpha^3 & 2^{n-k-2} & 2^{n-k-2} & \cdots & 2^{n-k-1}+\alpha^4 & \\
 & & & & & & & & & \\
J_{\binom{n}{2}\times 1} & & A_{\binom{n}{2}\times n} & & & & A_{\binom{n}{2}\times n} & & & B_{\binom{n}{2}\times\binom{n}{2}} \\
 & & & & & & & & & \\
 & & & & & & & & &
\end{array}\right]
\end{array}
$$

where

$$J_{\binom{n}{2}\times 1} = 2^{n-k-2} J_{\binom{n}{2}\times 1}$$

A has the same structure as A in Theorem 1.3 with 2^{n-k-2} instead of 1 and 2^{n-k-3} instead of 0

$M_{(2n+1)\times(2n+1)}$ will be used to represent the submatrix in the upper left-hand corner,

and $B_{\binom{n}{2}\times\binom{n}{2}}$ and $B^{-1}_{\binom{n}{2}\times\binom{n}{2}}$ have the pattern

B	B^{-1}	
2^{n-k-2}	$\dfrac{n^3-9n+12}{(n^3+2n^2-5n+2)2^{n-k-4}}$	if the column and row have two subscripts in common
2^{n-k-3}	$\dfrac{-n^2-n+8}{(n^3+2n^2-5n+2)2^{n-k-4}}$	if the column and row have one subscript in common
2^{n-k-4}	$\dfrac{2(n+3)}{(n^3+2n^2-5n+2)2^{n-k-4}}$	if the column and row have zero subscripts in common .

For the six interactions obtained with four variables, the pattern of B is:

$$\begin{array}{c|c}
 & \begin{array}{cccccc} 12 & 13 & 14 & 23 & 24 & 34 \end{array} \\
\begin{array}{c} 12 \\ 13 \\ 14 \\ 23 \\ 24 \\ 34 \end{array} &
\begin{bmatrix}
2^{n-k-2} & 2^{n-k-3} & 2^{n-k-3} & 2^{n-k-3} & 2^{n-k-3} & 2^{n-k-4} \\
2^{n-k-3} & 2^{n-k-2} & 2^{n-k-3} & 2^{n-k-3} & 2^{n-k-4} & 2^{n-k-3} \\
2^{n-k-3} & 2^{n-k-3} & 2^{n-k-2} & 2^{n-k-4} & 2^{n-k-3} & 2^{n-k-3} \\
2^{n-k-3} & 2^{n-k-3} & 2^{n-k-4} & 2^{n-k-2} & 2^{n-k-3} & 2^{n-k-3} \\
2^{n-k-3} & 2^{n-k-4} & 2^{n-k-3} & 2^{n-k-3} & 2^{n-k-2} & 2^{n-k-3} \\
2^{n-k-4} & 2^{n-k-3} & 2^{n-k-3} & 2^{n-k-3} & 2^{n-k-3} & 2^{n-k-2}
\end{bmatrix}
\end{array}$$

Simplifying, we obtain

$$\begin{vmatrix} M & \begin{matrix} J' \\ A' \\ A' \end{matrix} \\ J'A\ A & B \end{vmatrix} = |B| \begin{vmatrix} M - \begin{matrix} J' \\ A' \\ A' \end{matrix} [B]^{-1} [J\ A\ A] \end{vmatrix} ,$$

where $M_{(2n+1)\times(2n+1)}$ is a matrix whose elements are a function of α, B does not contain α and

$$\begin{bmatrix} J' \\ A' \\ A' \end{bmatrix} [B]^{-1} \quad [J\ A\ A]$$

has the form

$$\begin{vmatrix} c_1 & c_2J' & c_2J' \\ c_2J & c_3I + c_4JJ' & c_3I + c_4JJ' \\ c_2J & c_3I + c_4JJ' & c_3I + c_4JJ' \end{vmatrix}_{(2n+1) \times (2n+1)}$$

where c_1, c_2, c_3, and c_4 are constants independent of α. Thus, the $|X'X|$ reduces to

$$K_1 \begin{vmatrix} r & (s-\alpha)J' & (s+\alpha^2)J' \\ (s-\alpha)J & (\alpha^2+m)I+qJJ' & (-\alpha^3+m)I+qJJ' \\ (s+\alpha^2)J & (-\alpha^3+m)I+qJJ' & (\alpha^4+m)I+qJJ' \end{vmatrix}_{(2n+1) \times (2n+1)}$$

Use

$$\begin{vmatrix} D & B' \\ B & C \end{vmatrix} = |D| \; |C - B\,D^{-1}\,B'|$$

to reduce $|X'X|$ to:

$$K_2 \begin{vmatrix} aI + bJJ' & cI + dJJ' \\ cI + dJJ' & dI - fJJ' \end{vmatrix}_{2n \times 2n}$$

having determinant:

$$K_2(ae-c^2)^{n-1}\ ((a+nb)(e+nf) - (c+nd)^2)$$

where

$$a = \alpha^2 + m \qquad b = -\frac{\alpha^2}{r} + 2\frac{s}{r}\alpha - \frac{s^2}{r} + q$$

$$c = \alpha^4 + m \qquad d = \frac{\alpha^3}{r} - \frac{s}{r}\alpha^2 + \frac{s}{r}\alpha - \frac{s^2}{r} + q$$

$$e = -\alpha^3 + m \qquad f = -\frac{\alpha^4}{r} - 2\frac{s}{r}\alpha^2 - \frac{s^2}{r} + q$$

which upon substitution and multiplying out reduces to

$$|X'X| = K\,\alpha^{2n}\,(1+\alpha)^{2n}$$

where K is independent of α.

Thus the determinant is reduced to a constant times the result for a smallest composite design unsymmetric in the star points; so we have proved that the generalized variance decreases with increasing α, and that the optimal star point distance when the design is restricted to a hypercube having sides of length one is $1/(n+1)$.

1.6 Related Mathematical Results

1.6.1 Effects of linear transformations

In the $X_{N\times p}$ matrix if any column is multiplied by a constant k then the determinant will be multiplied by k^2. This is easily seen as the modified X matrix can be written as $X_{N\times p}\ P_{p\times p}$ where

$$P = \begin{vmatrix} I & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & I \end{vmatrix}$$

and

$$|P'X'X\ P| = |P'|\,|X'X|\ |P| = k^2\ |X'X|\ .$$

Multiplying a column in the design matrix X_D by k causes the following changes in the X matrix. The linear term is multiplied by k, the quadratic term is multiplied by k^2 and (n-1) interaction terms (for a full quadratic model) are multiplied by k; so this multiplies the determinant by $k^{2(n+2)}$. A result due to Hartley and Ruud [1969] is Theorem 1.6.1.

<u>Theorem 1.6.1</u>: If the n vectors X_t, are transformed to vectors z_t by

$$Z_t = X_t + \delta$$

where X_t is a row vector in the design matrix X_D or a row vector in the X matrix with $\delta_1 = 0$, then

$$|X'X| = |Z'Z| \ .$$

Proof: Z can be written as

$$Z_{N\times p} = X_{N\times p} \ A_{p\times p}$$

where

$$A = \begin{vmatrix} 1 & & & * \\ & 1 & & \\ & 0 & \ddots & \\ & & & 1 \end{vmatrix}$$

so

$$|A| = 1$$

thus

$$|Z'Z| = |A'| \ |X'X| \ |A| = |X'X| \ .$$

By combining the above results we can see how the determinant is changed by the usual linear transformations. For a particular example if each element of the design matrix $\mathcal{X}_D$, for a quadratic model, is transformed by $Z_{ij} = kx_{ij} + \delta_j$ then the determinant becomes

$$k^{2n(n+2)} \; |X'X| \quad .$$

1.6.2 The estimable terms in the model

Hartley [1959] discusses the terms in a model that can be estimated using a composite design. We will extend his result slightly using estimability considerations. We define estimability, give a standard theorem on estimability, then extend Hartley's result.

Definition: A linear function $\lambda'\beta$ is said to be linearly estimable $\Leftrightarrow \exists$ a vector $a_{N\times 1}$ such that $E(a'y) = \lambda'\beta$.

Theorem 1.6.2: $\lambda'\beta$ is estimable $\Leftrightarrow \lambda' = a'X$.

Proof: $\Rightarrow$

$\lambda'\beta$ is estimable $\Rightarrow \exists\, a \ni E(a'y) = \lambda'\beta$ but $E(a'y) = aX\beta \Rightarrow \lambda' = aX$.

$\Leftarrow$

$a'X = \lambda$ is a constant set of equations. Let a' be any solution, then

$$E(a'y) = a'X\beta = \lambda'\beta$$

Theorem 1.6.3:

(a) For a composite design symmetric in the star points it is always possible to estimate the following coefficients of a quadratic response surface:

The constant term, all linear coefficients, all quadratic coefficients, one of the product coefficients (interactions) selected from each of the alias sets.

(b) It is not possible to estimate more than one of the product coefficients from each alias set.

This theorem is an extension of Hartley's result in two ways:

(1) We allow main effects to be used in the defining contrast in the $(1/2^k)2^n$ fractional replicate, and

(2) We consider there to be 2^{n-k} alias sets by allowing the defining contrast to be counted as an alias set, Hartley allowed $2^{n-k} - 1$ alias sets.

Two simple examples using this extension are:

(1) A two variable composite design having seven points. This design uses a 2^{2-1} fractional factorial with alias structure I = AB.

(2) A three variable design having nine points with a 2^{3-2} fractional factorial with alias structure $I = A = BC = ABC$. This design allows the estimation of the constant term, three linear terms, three quadratic terms, and two of the three interaction terms, the BC interaction and either the AB or the AC interaction.

The experimenter must be careful when he is using highly fractionated designs. From each alias set one interaction term can be estimated, the choice of which interaction term to estimate is that of the experimenter. This choice can change the interpretation of the experiment.

Proof of Theorem 1.6.3.

From the center point and 2n star points we can find a vector such that $E(a'y) = \beta_i$ for the constant term, n linear terms, and n quadratic terms, 2n+1 terms in all. From the 2^{n-k} fractional factorial we can find 2^{n-k} estimable functions; the Yates algorithm will give us the estimable functions we desire. These functions will contain some combination of the following:

The constant term, main effects, two factor interactions, higher order interactions (which are not used in a quadratic model).

Since, if $\lambda_i\beta$ is estimable $\sum_i \lambda_i \beta$ is estimable, we can combine the λ's from the star with the λ's from the fractional factorial to estimate all terms in a model that picks only one interaction

term from each of the 2^{n-k} estimable functions of the fractional factorial. Note that 2^{n-k} may be greater or less than $\binom{n}{2}$ the number of interactions so we may have a saturated design or have many terms left over for estimating error. This completes part (a) of the theorem.

After noting that the 2n+1 star and center points make no contributions to the estimation of the interaction terms (for these points the row vector of the design matrix X_D has at most one non-zero element, thus for these rows all interaction elements of the X matrix are zero), we can immediately see that it is impossible to estimate more than one interaction term from each of the alias sets. This completes the proof of the theorem.

For composite designs unsymmetric in the star points a very similar theorems using the same method of proof is:

<u>Theorem 1.6.4</u>:

(a) For a composite design unsymmetric in the star points it is always possible to estimate the following coefficients of a quadratic response surface:

All quadratic terms and one coefficient from each of the 2^{n-k} alias sets.

(b) It is not possible to estimate more than one of the product coefficients from each of the alias sets.

A particular difference between composite designs symmetric in the star points and those unsymmetric in the star points is that an alias structure having words with three characters, e.g., I = ABC, allows the estimation of all terms in a quadratic response surface for the former design but not for the latter design. For the latter design note that if you use the principle block of the I = ABC alias structure the N design points in n dimensions project onto seven distinct points in three dimensions. With this alias structure the experimenter would commonly choose to estimate:

(a) The constant term, three linear terms, and three quadratic terms, or

(b) The constant term, three linear terms, and three interaction terms.

In case (b) you would be using the star points to estimate linear terms and the factorial structure to estimate the constant terms and the interaction terms.

In general such an alias structure would not be recommended, rather alias structures which have at least five characters for each word in the alias set, i.e., I = ABCDE, which allow the estimation of all terms in a quadratic response surface would be used.

1.6.3 Smallest fractional factorials - disproof of a conjecture

Using the alias structure I = ABC it is easy to construct composite designs symmetric in the star points for estimating all terms in a quadratic response surface. These designs use a 2^{n-k} fractional factorial with $k \le n/3$. It has been conjectured that k must be $\le n/3$ for all n, if all terms in a quadratic response surface are to be estimated. By enumeration of the possible alias structures it can be seen that the conjecture is true for $n \le 10$. These are the designs which are commonly used in practice. The conjecture is not true for all n, however. We disprove this conjecture by listing two different alias structures for $n = 11$, $k = 4$ that enable the estimation of all terms in a quadratic response surface. The first design has one three character alias word in the alias set, the second example has five or more characters for all words in the alias set. The second example can be found in Box and Hunter [1961]. We have underlined the words which we use to generate the alias structure.

Example 1.

I = ABCDE = ABFGH = CDFGI = ADEFHIJK = CDEFGH = ABEFGI = ABCDHI = EHI = BCFHIJK = BDEGIJK = ACGIJK = ACEGHJK = BDGHJK = BCEFJK = ADFJK

Example 2.

I = ABCGH = BCDEI = ACDFJ = ABCDEFGK = ADEGHI = BDFGHJ = ABEFIJ = CEFGHIJ = DEFHK = AFGIK = BEGJK = BCFHIK = ACEHJK = CDGIJK = ABDHIJK

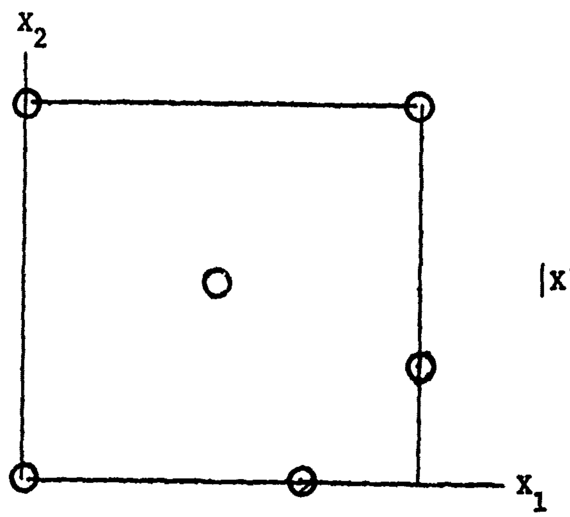
1.6.4 Optimum design-optimum composite design comparison

Figure 1.6.1 compares the optimal six point design obtained by Ruud [1969] with the optimal six point composite design. Both designs are restricted to a square with sides four units long. Ruud's design for estimating a quadratic response surface has $175. \times 10^5$ as the value of the determinant of the X'X matrix while the composite design has 20.7×10^5. The ratio of these two values is 8.45. A better comparison, perhaps, is the $2 \times p^{th}$ root of this ratio which is a measure of the ratio of the average standard deviation of a coefficient in the less efficient design to the standard deviation of a coefficient in the more efficient design. In this example with $p = 6$, $(8.45)^{1/12} = 1.195$. This increase in standard deviation reflects the penality paid in less precise estimates, for using the more easily obtained composite design rather than the optimal design obtained by solving a non-linear, non-convex program.

Note that the optimum composite design requires only three levels for each factor, while the Ruud design requires four levels for each factor. In fact we can observe that all optimum composite

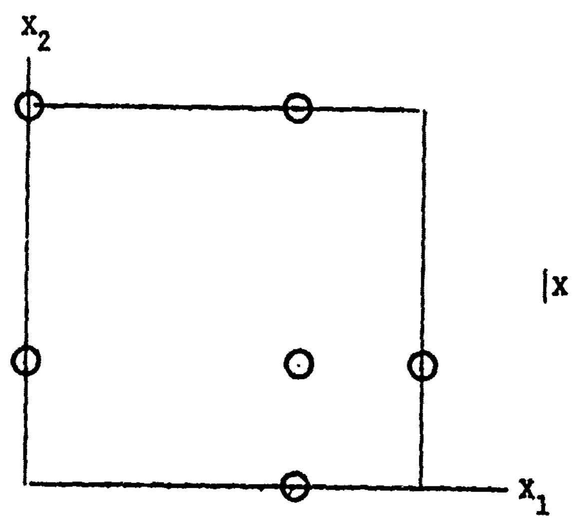
Figure 1.1

Six Point Design Comparison



$|X'X| = 175. \times 10^5$

Ruud's Six Point Design



$|X'X| = 20.7 \times 10^5$

Optimal Composite Design

designs on a hypercube require only three levels for each factor. This is extremely gratifying as in industrial experimentation the implementation of a factor level is often costly. Economic considerations might therefore indicate that an optimal composite design should be used rather than a more precise optimal design that requires more levels for each factor.

The use of an optimal composite design does not necessarily incur any penality at all. For example a nine point optimal design on a square is the same as a nine point composite design symmetric in the star points. These are the same as Kennard and Stone's [1969] and Box and Draper's [1971] optimal nine point design. All the above designs are 3^2 factorial designs having determinant 340×10^6 when the sides of the square have length four.

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APPENDIX

Some useful results about Matrices and Determinants:

Theorem [1]

$$\begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix}_{m \times n} = |A_{22}| \; |A_{11} - A_{12}A_{22}^{-1}A_{21}|$$

when A_{22} is square and non-singular.

Proof: Theorem 1.50, Graybill [1961].

Theorem [2]

$$(I + AB)^{-1} = (I - A(I+BA)^{-1}B)$$

Proof: Multiply out to verify.

Theorem [3]

$$|I + AB| = |I + BA|$$

Proof: Consider $\begin{vmatrix} I_J & B \\ -A & I_K \end{vmatrix}$ and use Theorem [1] twice to obtain

$$\begin{vmatrix} I_J & B \\ -A & I_K \end{vmatrix} = |I_K| \; |I_J + BI_K^{-1}A| = |I_J| \; |I_K + AI_J^{-1}B| \quad .$$

Theorem [4]

$$|aI + bJJ'|_{n\times n} = a^{n-1}(a + nb)$$

Proof:

$$|aI + bJJ'| = a^n \; |I + \frac{b}{a}JJ'|$$

$$= a^n \; |1 + \frac{b}{a}J'J| \text{ by Theorem [3]}$$

$$= a^n(1+\frac{nb}{a}) = a^{n-1}(a + nb)$$

Theorem [5]

$$[aI + bJJ']^{-1}_{n\times n} = [cI + dJJ']_{n\times n}$$

where $c = \frac{1}{a}$ and $d = -\frac{b}{a(a+nb)}$.

Proof: Multiply out.

Theorem [6]

$$\begin{vmatrix} aI + bJJ' & cI + dJJ' \\ cI + dJJ' & eI + fJJ' \end{vmatrix}_{2n\times 2n} = (ae-c^2)^{n-1}\,[(a+nb)(e+nf) - (c+nd)^2]$$

Proof:

$$\begin{vmatrix} aI + bJJ' & cI + dJJ' \\ cI + dJJ' & eI + fJJ' \end{vmatrix} = a^{n-1}(a+nb)\,\Big|[eI + fJJ'] - [cI + dJJ']$$

$$[\frac{1}{a}I - \frac{b}{a(a+nb)}\,JJ'][cI + dJJ']\Big|$$

$$= a^{n-1}(a+nb)\,\Big|\Big(e - \frac{c^2}{a}\Big)I + \Big\{f - \frac{2cd}{a}\ \frac{bc^2}{a(a+nb)}$$

$$- \frac{nbcd}{a(a+nb)} - n\Big(\frac{d^2}{a} + \frac{bcd}{a(a+nb)} + \frac{nbd^2}{a(a+nb)}\Big)\Big\}JJ'\Big|$$

$$= a^{n-1}(a+nb)\Big(e - \frac{c^2}{a}\Big)^{n-1}\Big\{e - \frac{c^2}{a} + nf - \frac{2ncd}{a}$$

$$- \frac{nd^2}{a} + \frac{nb}{a(a+nb)}\,(c^2 + 2ncd + n^2b^2)\Big\}$$

$$= (ae-c^2)^{n-1}\,\{(a+nb)(e+nf) - (c+nd)^2\}\ .$$